

Supplemental Table 1. The detail of 1510 features extracted by PyRadiomics.

Features	Total
Shape features	14
First-order features	18
Gray-level co-occurrence matrix features	24
Gray-level run-length matrix features	16
Gray-level size zone matrix features	16
Gray-level dependence matrix features	14
Log sigma features	264
Wavelet features	704
square features	88
square root features	88
logarithm features	88
exponential features	88
gradient features	88
Total	1510

Information of these features and the formulas for calculating them can be found in the documentation of PyRadiomics (<https://pyradiomics.readthedocs.io/en/latest/features.html>).

Supplemental Table 2. Classifier and feature selector or decomposition method included in TPOT.

Classifier	Feature selector or decomposition method
Gaussian naive Bayes	Select the p-values corresponding to the family-wise error rate (SelectFwe)
Bernoulli naive Bayes	Select features according to a percentile of the highest scores (SelectPercentile)
Multinomial naive Bayes	Feature selector that removes all low-variance features (VarianceThreshold)
Decision tree	Feature ranking with recursive feature elimination (RFE)
Extra trees	Meta-transformer for selecting features based on importance weights (SelectFromModel)
Random forest	Fast algorithm for independent component analysis (FastICA)
Gradient boosting	Principal component analysis (PCA)
K-nearest neighbors	
Linear support vector classification	
Logistic regression	
Extreme gradient boosting	
Stochastic gradient descent	
Multi-layer perceptron	

TPOT (version 0.23.2) based on scikit-learn (version 0.23.2) were used in this study.

Supplemental Table 3. Pipelines in the tree-based pipeline optimization tool using combination of contrast-enhanced T1 weighted and T2 weighted features.

Pipeline	Feature selector	Number of selected features	Transformer	Classifier
1	VarianceThreshold	624	MinMaxScaler	
2	RFE	466	OneHotEncoder	
3	RFE	466	OneHotEncoder	
4	RFE	466	MaxAbsScaler	
5	RFE	466	MinMaxScaler	GradientBoosting
6	RFE	466	RobustScaler	
7	RFE	466	OneHotEncoder	
8	VarianceThreshold	622	RobustScaler	
9	RFE	466	StandardScaler	
10	RFE	466	MinMaxScaler	

Abbreviation: RFE, Feature ranking with recursive feature elimination.

Supplemental Table 4. Details of the 149 key features.

Contrast-enhanced T1-weighted features	T2-weighted features
Original features	
original_firstorder_Kurtosis	original_glcm_Imc2
original_firstorder_Median	original_gldm_DependenceVariance
original_firstorder_Skewness	original_glrlm_GrayLevelNonUniformity
original_shape_Elongation	original_glrlm_LongRunLowGrayLevelEmphasis
original_shape_Sphericity	original_glrlm_RunLengthNonUniformity
	original_shape_Flatness
Exponential features	
exponential_firstorder_RootMeanSquared	exponential_firstorder_Kurtosis
	exponential_glrlm_GrayLevelNonUniformity
Gradient features	
gradient_firstorder_InterquartileRange	gradient_glrlm_RunLengthNonUniformity
gradient_glszm_GrayLevelNonUniformity	
Logarithm features	
logarithm_firstorder_Maximum	logarithm_glc当地Entropy
logarithm_firstorder_Mean	logarithm_firstorder_Range
logarithm_firstorder_Median	logarithm_firstorder_Uniformity
logarithm_firstorder_RootMeanSquared	logarithm_glc当地Autocorrelation
logarithm_glrlm_ShortRunHighGrayLevelEmphasis	logarithm_glc当地ClusterTendency
logarithm_glszm_LowGrayLevelZoneEmphasis	logarithm_glc当地DifferenceEntropy
	logarithm_glc当地Imc2
	logarithm_glc当地JointAverage
	logarithm_glc当地JointEnergy
	logarithm_glc当地JointEntropy
	logarithm_glc当地SumAverage
	logarithm_glc当地SumEntropy
	logarithm_glc当地SumSquares
	logarithm_gldm_GrayLevelVariance
	logarithm_gldm_HighGrayLevelEmphasis
	logarithm_glrlm_GrayLevelNonUniformity
	logarithm_glrlm_LongRunLowGrayLevelEmphasis
	logarithm_glrlm_ShortRunEmphasis
	logarithm_glszm_HighGrayLevelZoneEmphasis
Log-sigma features	
log-sigma-3-0-mm-3D_glrlm_LongRunLowGrayLevelEmphasis	log-sigma-3-0-mm-3D_firstorder_90Percentile
log-sigma-3-0-mm-3D_glrlm_RunVariance	log-sigma-3-0-mm-3D_firstorder_Kurtosis
log-sigma-4-0-mm-3D_firstorder_Skewness	log-sigma-3-0-mm-3D_firstorder_Maximum
log-sigma-4-0-mm-3D_glrlm_ShortRunEmphasis	log-sigma-3-0-mm-3D_firstorder_Skewness
log-sigma-5-0-mm-3D_glrlm_ShortRunEmphasis	log-sigma-3-0-mm-3D_glrlm_HighGrayLevelRunEmphasis
	log-sigma-4-0-mm-3D_firstorder_Maximum
	log-sigma-4-0-mm-3D_gldm_GrayLevelNonUniformity

	log-sigma-4-0-mm-3D_glrlm_HighGrayLevelRunEmphasis
	log-sigma-5-0-mm-3D_firstrorder_Maximum
	log-sigma-5-0-mm-3D_firstrorder_Range
	log-sigma-5-0-mm-3D_gldm_DependenceNonUniformity
	log-sigma-5-0-mm-3D_gldm_DependenceVariance
	log-sigma-5-0-mm-3D_gldm_GrayLevelNonUniformity
Square features	
	square_gldm_LargeDependenceHighGrayLevelEmphasis
	square_glrlm_GrayLevelNonUniformity
Squareroot features	
squareroot_firstrorder_Mean	squareroot_firstrorder_Entropy
squareroot_firstrorder_Median	squareroot_firstrorder_Range
squareroot_firstrorder_RootMeanSquared	squareroot_glcg_Imc2
	squareroot_glcg_JointAverage
	squareroot_glcg_JointEntropy
	squareroot_glcg_SumAverage
	squareroot_glcg_SumEntropy
	squareroot_gldm_HighGrayLevelEmphasis
	squareroot_gldm_LargeDependenceLowGrayLevelEmphasis
	squareroot_glrlm_GrayLevelNonUniformity
	squareroot_glrlm_LongRunLowGrayLevelEmphasis
	squareroot_glszm_GrayLevelVariance
	squareroot_glszm_HighGrayLevelZoneEmphasis
Wavelet features	
wavelet-HLL_firstrorder_10Percentile	wavelet-HHH_gldm_DependenceEntropy
wavelet-HLL_firstrorder_90Percentile	wavelet-HHH_glrlm_ShortRunHighGrayLevelEmphasis
wavelet-HLL_firstrorder_InterquartileRange	wavelet-HHH_glszm_GrayLevelNonUniformity
wavelet-HLL_firstrorder_Maximum	wavelet-HHL_firstrorder_10Percentile
wavelet-HLL_firstrorder_MeanAbsoluteDeviation	wavelet-HHL_firstrorder_90Percentile
wavelet-HLL_firstrorder_Minimum	wavelet-HHL_firstrorder_InterquartileRange
wavelet-HLL_firstrorder_Range	wavelet-HHL_firstrorder_MeanAbsoluteDeviation
wavelet-HLL_firstrorder_RobustMeanAbsoluteDeviation	wavelet-HHL_firstrorder_RobustMeanAbsoluteDeviation
wavelet-HLL_firstrorder_Variance	wavelet-HHL_glrlm_ShortRunHighGrayLevelEmphasis
wavelet-HLL_glrlm_LowGrayLevelRunEmphasis	wavelet-HHL_glszm_SmallAreaEmphasis
wavelet-LLL_firstrorder_Kurtosis	wavelet-HLH_gldm_DependenceNonUniformity
wavelet-LLL_firstrorder_Mean	wavelet-HLH_glszm_SizeZoneNonUniformity
wavelet-LLL_firstrorder_RootMeanSquared	wavelet-HLH_glszm_SmallAreaLowGrayLevelEmphasis
wavelet-LLL_firstrorder_Skewness	wavelet-HLL_glcg_Autocorrelation
wavelet-LLL_glcg_Contrast	wavelet-HLL_glcg_JointAverage
wavelet-LLL_glcg_DifferenceAverage	wavelet-HLL_glcg_SumAverage
wavelet-LLL_glcg_DifferenceEntropy	wavelet-HLL_gldm_LowGrayLevelEmphasis
wavelet-LLL_glcg_DifferenceVariance	wavelet-HLL_glszm_GrayLevelNonUniformity
wavelet-LLL_glcg_Id	wavelet-HLL_glszm_SizeZoneNonUniformity

wavelet-LLL_glcM_Idm	wavelet-HLL_glszm_ZoneEntropy
wavelet-LLL_glcM_InverseVariance	wavelet-LHH_glszm_SizeZoneNonUniformity
wavelet-LLL_gldm_DependenceNonUniformityNormalized	wavelet-LHL_firstorder_Maximum
wavelet-LLL_gldm_LargeDependenceEmphasis	wavelet-LHL_firstorder_Minimum
wavelet-LLL_grlm_RunLengthNonUniformity	wavelet-LHL_firstorder_Range
	wavelet-LHL_firstorder_Skewness
	wavelet-LHL_glcM_ClusterShade
	wavelet-LHL_grlm_LongRunHighGrayLevelEmphasis
	wavelet-LHL_glszm_GrayLevelNonUniformity
	wavelet-LHL_glszm_HighGrayLevelZoneEmphasis
	wavelet-LHL_glszm_LowGrayLevelZoneEmphasis
	wavelet-LHL_glszm_SizeZoneNonUniformity
	wavelet-LHL_glszm_ZoneEntropy
	wavelet-LLH_glcM_Autocorrelation
	wavelet-LLH_glcM_JointAverage
	wavelet-LLH_glcM_JointEnergy
	wavelet-LLH_glcM_MaximumProbability
	wavelet-LLH_glcM_SumAverage
	wavelet-LLH_glcM_SumEntropy
	wavelet-LLH_gldm_DependenceVariance
	wavelet-LLH_gldm_HighGrayLevelEmphasis
	wavelet-LLH_grlm_HighGrayLevelRunEmphasis
	wavelet-LLH_grlm_RunLengthNonUniformity
	wavelet-LLL_glcM_Imc2
	wavelet-LLL_grlm_LowGrayLevelRunEmphasis
	wavelet-LLL_grlm_ShortRunLowGrayLevelEmphasis
	wavelet-LLL_glszm_HighGrayLevelZoneEmphasis
	wavelet-LLL_glszm_ZoneEntropy

Abbreviations: glcm, gray-level co-occurrence matrix; grlm, gray-level run-length matrix; glszm, gray-level size zone matrix; gldm, gray-level dependence matrix.

Supplemental Table 5. Definition of the metrics.

Metrics	Definition
Accuracy	$(TP+TN)/(TP+TN+FP+FN)$
Precision	$TP/(TP+FP)$
Specificity	$TN/(TN+FP)$
Sensitivity	$TP/(TP+FN)$
AUC	Areas under the receiver operating characteristic curve

Abbreviations: TP, true positive; TN, true negative; FP, false positive; FN, false negative.